



ACTIVITIES OF **J**OINT
USAGE/**R**ESEARCH
CENTER

JURC Cooperative Research Subjects 2011

(1 April 2011 ~ 31 March 2012)

STARTING-UP SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

High-energy Ion Generation through the Interactions of Laser with Nano Particles

NAKAI, Mitsuo, Institute of Laser Engineering, Osaka University
Host in JURC TOKITA, Shigeki

Development and Application of Time-resolved Irradiation Method by Cooled Ion Beams

NODA, Koji, National Institute of Radiological Sciences
Host in JURC NODA, Akira

Optical and Electrical Properties of Mixed Organic Semiconductors

NAITO, Hiroyoshi, The School of Engineering, Osaka Prefecture University

Host in JURC KANEMITSU, Yoshihiko

Preparation of High-Performance Polycarbonate/Transition-Metal-Complex Hybrid Materials

KONISHI, Gen-ichi, Graduate School of Engineering, Tokyo Institute of Technology

Host in JURC OZAWA, Fumiyuki

Synthesis of Sugar-Acetylenes by Iron-Catalyzed Cross-Coupling and Study on Their Stimulus-Response Luminescence

ORITA, Masahiro, Faculty of Engineering, Okayama University of Science

Host in JURC NAKAMURA, Masaharu

Development of Negative Thermal Expansion Material Based on a Perovskite BiNiO_3

AZUMA, Masaki, Materials and Structures Laboratory, Tokyo Institute of Technology

Host in JURC SHIMAKAWA, Yuichi

Development of Novel 3-Dimensional π -Extended Molecules Directed toward Electronic Materials

SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University

Host in JURC MURATA, Yasujiro

Metagenome and Metatranscriptome Analysis of Soil Microbial Diversity and Functions in Natural and Degraded Tropical Rainforests

HARADA, Ko, Department of Forest Resources, Faculty of Agriculture, Ehime University

Host in JURC GOTO, Susumu

Integrated Analysis for Text Data and High Throughput Data Related to Metabolic Pathways

YONEZAWA, Akinori, Database Center for Life Science, Research Organization of Information and Systems

Host in JURC KANEHISA, Minoru

Efficient Search Algorithms for Structured Data in Bioinformatics

TAKASU, Atsuhiko, Digital Content and Media Sciences Research Division, National Institute of Informatics

Host in JURC AKUTSU, Tatsuya

Probabilistic Methods for Analysis on Protein Interaction Networks

MARUYAMA, Osamu, Institute of Mathematics for Industry, Kyushu University

Host in JURC AKUTSU, Tatsuya

Finding Frequent Similar Regions from Genome Sequences

NAKAMURA, Atsuyoshi, Graduate School of Information Science and Technology, Hokkaido University

Host in JURC MAMITSUKA, Hiroshi

Study of Functional Optical Thin Films by Sol-gel Method

IHARA, Rie, Department of Applied Physics, Tohoku University

Host in JURC MASAI, Hirokazu

Correlation of Structure and Electronic Structure in Thin Films of Group 10 Metals Dione-Dioximate

TAKEDA, Keiki, Graduate School of Engineering, Muroran Institute of Technology

Host in JURC SATO, Naoki

Structural Change of Frustrated Polymer Crystal at Low Temperature

OKIHARA, Takumi, Graduate School of Natural Science and Technology, Okayama University

Host in JURC TOSAKA, Masatoshi

Investigation of Extraction Behaviors of Metal Ions in Liquid-liquid Extraction Systems Using a Novel Multidentate Ligand

MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education

Host in JURC SOHRIN, Yoshiki

A New Soft-Interface Built of Stereocontrolled Hydrophilic Polymers

KATSUMOTO, Yukiteru, Graduate School of Science, Hiroshima University

Host in JURC HASEGAWA, Takeshi

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

X-Ray Structure Analysis of Reaction Mechanism of Catabolic Enzymes

OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University

Host in JURC HATA, Yasuo

X-Ray Structural Studies on Cold Adaptation of Proteins from Psychrophiles

GOUGAMI, Yoshitaka, Organization for Research and Development of Innovative Science and Technology, Kansai University

Host in JURC HATA, Yasuo

Multi-dimensional Doppler Laser Cooling for Realization of Ultralow-temperature Ion Beam

ITO, Kiyokazu, Graduate School of Advanced Sciences of Matter, Hiroshima University

Host in JURC NODA, Akira

Photocarrier Recombination Dynamics in Nanodomain-structured Ferroelectrics
FUNAKUBO, Hiroshi, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology
Host in JURC KANEMITSU, Yoshihiko

Design and Synthesis of Metal Ligands which Facilitate the Reductive Elimination Reaction and Their Application to the Synthesis of Cycloparaphenylenes
KORENAGA, Toshinobu, Graduate School of Natural Science and Technology, Okayama University
Host in JURC YAMAGO, Shigeru

Effective Transformation of Carbon-Resources on Dynamic Tetrairon Cores
OKAZAKI, Masaaki, Graduate School of Science and Technology, Hirosaki University
Host in JURC OZAWA, Fumiyuki

Development of Efficient Iron Catalysts for Selective Carbon-carbon Bond Forming Reactions Based on Mechanistic Studies
NAGASHIMA, Hideo, Institute for Materials Chemistry and Engineering, Kyushu University
Host in JURC NAKAMURA, Masaharu

Development of Methods for Discrimination and Syntheses of Chiral Molecules with Phosphoroselenic Acid Derivatives Bearing a Binaphthyl Group
MURAI, Toshiaki, Faculty of Engineering, Gifu University
Host in JURC TOSHIMITSU, Akio

Efficient Construction of Polyfunctionalized Molecules by Cooperative Effect of Transition Metals and Heteroatoms
SEGI, Masahito, School of Chemistry, College of Science and Engineering, Kanazawa University
Host in JURC TOSHIMITSU, Akio

Prediction of Enzymatic Function of Cytochromes P450 Involved in Steroid Biosynthesis and Metabolism
OHNISHI, Toshiyuki, Division of Global Research Leaders, Shizuoka University
Host in JURC WATANABE, Bunta

Comprehensive Analysis of Calpain Substrate Specificity by the Integrated Data-mining Method
ONO, Yasuko, Tokyo Metropolitan Institute of Medical Science
Host in JURC MAMITSUKA, Hiroshi

Allele-specific Repertoire Overlap Analyzed by an HLA-binding Peptide Prediction Algorithm
UDAKA, Keiko, Kochi Medical School
Host in JURC MAMITSUKA, Hiroshi

Study on the Fabrication Process of Organic-inorganic Hybrid Materials
FUJINO, Shigeru, Department of Chemical Engineering, Faculty of Engineering, Kyusyu University
Host in JURC YOKO, Toshinobu

Cornea Regeneration by Small Molecule Fibronectin
KOIZUMI, Noriko, Faculty of Life and Medical Science, Doshisha University
Host in JURC UESUGI, Motonari

Development of a Technology for Solubilizing C₆₀ Fullerene Encapsulating an Atom(s) into Aqueous Solution
MURAKAMI, Masahiro, Department of Pharmacy, Osaka Ohtani University
Host in JURC MURATA, Yasujiro

Concentrated Polymer Brushes with Glucose-Sensing Ability
YOSHIKAWA, Chiaki, WPI-MANA, National Institute for Materials Science
Host in JURC TSUJII, Yoshinobu

Development of Novel Electrolyte for PEFC (Polymer Electrolyte Fuel Cell) by Living Radical Polymerization
MORINAGA, Takashi, Department of Chemistry Mechanical Engineering, Tsuruoka National College of Technology
Host in JURC TSUJII, Yoshinobu

Skin Permeation Using Arginine-rich Peptides
KOGURE, Kentaro, Kyoto Pharmaceutical University
Host in JURC FUTAKI, Shiroh

Time-resolved Grazing Incidence Small Angle X-ray Scattering for Dewetting in Polymer Blend Thin Films
OGAWA, Hiroki, Japan Synchrotron Radiation Institute
Host in JURC KANAYA, Toshiji

Studies on Crystal Structure and Formation Process of Poly(lactic acid)
KAWAI, Takahiko, Division of Production Science and Technology, Graduate School of Engineering, Gunma University
Host in JURC KANAYA, Toshiji

Making of the Vertical Cross Section of Bioactive Trace Metals in the Japan Sea
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kinki University
Host in JURC SOHRIN, Yoshiki

Electronic and Molecular Analysis of Biophysical and Biochemical Processes through Combined Quantum-Chemical/Statistical-Mechanical Approach
TAKAHASHI, Hideaki, Department of Chemistry, Graduate School of Science, Tohoku University
Host in JURC MATUBAYASI, Nobuyuki

Study of Dynamic Heterogeneity in Multi-Component Polymer Systems in Miscible State
URAKAWA, Osamu, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

STARTING-UP SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Optical Functionalities of Silicon Photonic Crystals
TAKAHASHI, Yasushi, Research Organization for the 21st Century, Osaka Prefecture University
Host in JURC KANEMITSU, Yoshihiko

Structure and Function of a Novel FADH₂-dependent Dehalogenase
KURATA, Atsushi, Department of Applied Biological Chemistry, Faculty of Agriculture, Kinki University
Host in JURC KURIHARA, Tatsuo

Preparation, Structure and Electronic Properties of Thin Films of Furan-Fused Polycyclic Aromatic Compounds
HAYASHI, Naoto, Graduate School of Science and Engineering for Research, University of Toyama
Host in JURC SATO, Naoki

Physics of THz Generation through the Interactions of Laser with Clusters
NAGASHIMA, Takeshi, Institute of Laser Engineering, Osaka University
Host in JURC HASHIDA, Masaki

Studies on Peculiar Changes in Higher-order Crystalline Lamellar Structures of Poly(ethylene glycol) upon Heating
SAKURAI, Shinichi, Biobased Materials Science, Graduate School of Science and Technology, Kyoto Institute of Technology
Host in JURC TOSAKA, Masatoshi

Development of Organic Solar Cell via the Interplay of Nanocarbon Science and Main Group Element Chemistry
TAJIMA, Tomoyuki, Graduate School of Environmental Science, Okayama University
Host in JURC TOKITOH, Norihiro

Domain Wall Oscillator by Spin Current
NAKATANI, Yoshinobu, Graduate School of Informatics and Engineering, University of Electro-Communications
Host in JURC ONO, Teruo

Study for Tunnel Magnetoresistive Effect and Local Magnetism of Magnetic Tunnel Junctions Using Co₂MnSn Heusler Alloy Electrodes Prepared by Atomically-controlled Alternate Deposition
TANAKA, Masaaki, Department of Engineering Physics, Electronics and Mechanics, Nagoya Institute of Technology
Host in JURC ONO, Teruo

Small Molecules that Promote Differentiation into Pancreatic β Cells
KUME, Shouen, Institute of Molecular Embryology and Genetics, Kumamoto University
Host in JURC UESUGI, Motonari

Study on the Regulatory Mechanism of Plant Epidermal Cell Differentiation
TOMINAGA, Rumi, Interdisciplinary Research Organization, University of Miyazaki
Host in JURC AOYAMA, Takashi

Overexpression of Miraculin Using *Arabidopsis thaliana*
INOUE, Hiroyasu, Faculty of Human Life and Environment
Host in JURC AOYAMA, Takashi

Synthesis and Functions of Multi-Bridged Naphthalene Oligomers
KURAMOCHI, Koji, Graduate School of Life and Environmental Sciences, Kyoto Prefectural University
Host in JURC KAWABATA, Takeo

Search for New Method to Prepare Photovoltaic Device Using Reformed Coal Mixture
YAMASHITA, Makoto, Department of Applied Chemistry, Faculty of Science and Engineering, Chuo University
Host in JURC MURATA, Yasujiro

Development of Supramolecular Multimetallic Catalyst for Selective Degradation of Lignins
WATANABE, Takashi, Research Institute for Sustainable Humanosphere, Kyoto University
Host in JURC NAKAMURA, Masaharu

Dynamics in the Interaction between Arginine-rich Peptides and Biomembranes
KOBAYASHI, Toshihide, ASI RIKEN
Host in JURC FUTAKI, Shiroh

Spin and Nuclear Spin Generation in Semiconductors by an Electrical Way
NITTA, Junsaku, Department of Materials Science, Tohoku University
Host in JURC KOBAYASHI, Kensuke

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Studies on the Transport and Metabolism of the Essential Trace Element Selenium in Mammals
MIHARA, Hisaaki, Department of Biotechnology, College of Life Sciences, Ritsumeikan University
Host in JURC KURIHARA, Tatsuo

The Control of the Antiphase Boundary in Ferrimagnetic Spinel Ultrathin Films
NAGAHAMA, Taro, Graduate School of Engineering, Hokkaido University
Host in JURC ONO, Teruo

Highly Efficient Synthesis of π -Conjugated Polymers via Direct Arylation
KANBARA, Takaki, Graduate School of Pure and Applied Sciences, Tsukuba Research Center for Interdisciplinary Materials Science, University of Tsukuba
Host in JURC OZAWA, Fumiyuki

Development of Induction Systems in Plants Using Caged Chemicals
HAYASHI, Ken-ichiro, Department of Biochemistry, Okayama University of Science
Host in JURC AOYAMA, Takashi

Search for Biologically Active Compounds from a Synthetic Library of Nitrogen Heterocycles with Chiral Tetrasubstituted Carbon
ISHIBASHI, Masami, Graduate School of Pharmaceutical Sciences, Chiba University
Host in JURC KAWABATA, Takeo

Spectroscopic Study of the Influence of Gold on a Hierarchical Two-dimensional Molecular Aggregate of Supramolecules
YAMADA, Norihiro, Graduate School of Education, Chiba University
Host in JURC HASEGAWA, Takeshi

Dynamics in Physical Network Formed through Aggregation
SHIKATA, Toshiyuki, Graduate School of Science, Osaka University
Host in JURC MASUBUCHI, Yuichi

Development of Novel Electronic Phase Materials in Complex Iron-titanium Oxides
FUJII, Tatsuo, Faculty of Engineering, Okayama University
Host in JURC SAITO, Takashi

SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Manipulation of π -conjugated Polymers by a Scanning Tunneling Microscope Tip
TAKAJO, Daisuke, Graduate School of Science, Osaka University
Host in JURC KURATA, Hiroki

Electron Spectroscopic Study of Degradation of Optical Properties in First Mirror Materials for Fusion Plasma Diagnostics
MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science and Engineering, Shimane University
Host in JURC KURATA, Hiroki

NMR Characterization of Carbon Nitride
TAKARABE, Kenichi, Department of Applied Science, Okayama University of Science
Host in JURC KAJI, Hironori

Solid-State NMR Analysis of Molecular Orientation in Organic LED Materials
ADACHI, Chihaya, OPERA, Kyushu University
Host in JURC KAJI, Hironori

Solid-state-NMR Study on Luminescence and Structure Characteristics of Organic Molecules
TOKUDOME, Yasuaki, Graduate School of Engineering, Osaka Prefecture University
Host in JURC KAJI, Hironori

Systematic Syntheses and Properties of Polycyclic Aromatics Containing a Phosphorus Atom
OKUMA, Kentaro, Department of Chemistry, Faculty of Science, Fukuoka University
Host in JURC SASAMORI, Takahiro

Synthesis and Structure of Transition Metal Complexes with New Tripodal Tetradentate Ligand
UNNO, Masafumi, Graduate School of Engineering, Gunma University
Host in JURC TOKITOH, Norihiro

Physicochemical Properties of Novel Aromatic Compounds with Heteroatoms
SAITO, Masaichi, Department of Chemistry, Graduate School of Science and Engineering, Saitama University
Host in JURC TOKITOH, Norihiro

SUBJECTS ENCOURAGING JOINT PROGRAM

GEOTRACES JAPAN Symposium
GAMO, Toshitaka, Atmosphere and Ocean Research Institute, The University of Tokyo
Host in JURC SOHRIN, Yoshiki

The 7th International Workshop for East Asian Young Rheologists
SAKURAI, Shinichi, The Center for Fiber and Textile Science, Kyoto Institute of Technology
Host in JURC WATANABE, Hiroshi

Investigation on the Electronic States of Transition Metal Oxides Containing Unusually High-valent Cations
KAWAKAMI, Takateru, Institute of Quantum Science, Nihon University
Host in JURC SHIMAKAWA, Yuichi

JURC Publications

(until 31 May 2011)

A Clique-based Method for the Edit Distance between Unordered Trees and Its Application to Analysis of Glycan Structures

Fukagawa, D.; Tamura, T.; Takasu, A.; Tomita, E.; Akutsu, T., *BMC Bioinformatics*, **12**(Suppl 1), S13 (2011).

Abstract

This paper presents a practical method for computing the edit distance between rooted unordered trees. In this method, the original edit distance problem is transformed into the maximum clique problem and then efficient solvers for the maximum clique problem are applied. The proposed method was applied to similar structure search for glycan structures and the result suggests that the proposed method can efficiently compute the edit distance for moderate size unordered trees.

Algorithms for Finding a Minimum Repetition Representation of a String

Nakamura, A.; Saito, T.; Takigawa, I.; Mamitsuka, H.; Kudo, M., *LNCS 6393 (Proc. of SPIRE 2010)*, 185-190 (2010).

Abstract

A string with many repetitions can be written compactly by replacing h -fold contiguous repetitions of substring r with $(r)^h$. We refer to such a compact representation as a *repetition representation string* or RRS, by which a set of disjoint or nested tandem arrays can be compacted. In this paper, we study the problem of finding a *minimum RRS* or MRRS, where the size of an RRS is defined to be the sum of its component letter sizes and the sizes needed to describe the repetitions $(\bullet)^h$ which are defined as $w_R(h)$ using a repetition weight function w_R . We develop two dynamic programming algorithms to solve the problem. One is CMR that works for any repetition weight function, and the other is CMR-C that is faster but can be applied only when the repetition weight function is constant. CMR-C is an $O(w(n+z))$ -time algorithm using $O(n+z)$ space for a given string with length n , where w and z are the number of distinct primitive tandem repeats and the number of their occurrences, respectively. Since $w = O(n)$ and $z = O(n \log n)$ in the worst case, CMR-C is an $O(n^2 \log n)$ -time $O(n \log n)$ -space algorithm, which is faster than CMR by $((\log n)/n)$ -factor.

Enhanced Adsorption and Fluorescence Efficiency of Silylethynyl-functionalized Oligothiophenes and Thieno[3,2-*b*]thiophene

Asai, K.; Konishi, G.; Nakajima, Y.; Kawachi, S.; Ozawa, F.; Mizuno, K., *Journal of Organometallic Chemistry*, **696**, 1266-1271 (2011).

Abstract

We synthesized silylethynyl-substituted oligothiophenes and thieno[3,2-*b*]thiophenes by the palladium-catalyzed Sonogashira coupling reaction. These compounds exhibit longer absorbance and fluorescence peak wavelengths, higher absorption coefficients, and higher quantum efficiency than their corresponding unsubstituted molecules and *tert*-butylethynyl derivatives. From the DFT calculation, the energy band gap between HOMO and LUMO decreases by the introduction of a silicon atom. Thus, silyl groups can play important role in enhancing the quantum efficiency and decreasing the band-gap of chromophores. Hence, silylethynyl group can serve as a highly efficient auxiliary for use in optical devices.

Entanglement Dynamics in Miscible Polyisoprene/Poly(*p*-tert-butylstyrene) Blends

Watanabe, H.; Chen, Q.; Kawasaki, Y.; Matsumiya, Y.; Inoue T.; Urakawa, O., *Macromolecules*, **44**, 1570-1584 (2011).

Abstract

Viscoelastic, dielectric, and rheo-optical behavior was examined for miscible blends of high- M *cis*-polyisoprene (PI) and poly(*p*-*tert*-butylstyrene) (PtBS). The slow dielectric relaxation of the blends was exclusively attributed to the global motion of the PI chains having the type-A dipoles. The PI and PtBS chains behaved as the fast and slow (low- and high-friction) components and were well entangled with each other. The dynamics of these chains changed significantly with temperature T . At high T , the blend exhibited two-step entanglement plateau of the storage modulus $G'(\omega)$, and the plateaus at high and low angular frequencies (ω) were attributed, with the aid of the dielectric data, to the entanglement among all component chains and that between the PtBS chains, respectively. The entanglement length a characterizing the high- ω plateau was well described by a simple mixing rule based on the number fraction n of the Kuhn segments of the components, $a = n_{PI}a_{PI}^{bulk} + n_{PtBS}a_{PtBS}^{bulk}$. This result was consistent with the current molecular picture relating the entanglement density to the packing length p ($\approx a/20$). The complex moduli G^* of the blends in the high- ω plateau zone were well described by a simple blending law combined with this mixing rule of a , which was consistent with the rheo-optical data. At low T , the blend exhibited the Rouse-like power-law behavior of storage and loss moduli, $G' = G'' \propto \omega^{1/2}$, in the range of ω where the high- ω plateau was supposed to emerge. This lack of the high- ω plateau was attributed to retardation of the Rouse equilibration of the PI chain over the entanglement length a due to the hindrance from the slow PtBS chains: The PI and PtBS chains appeared to be equilibrated *cooperatively/simultaneously* at a rate essentially determined by PtBS. The Rouse equilibration time, evaluated from the G^* data of the blend, was just moderately shorter than the dielectrically determined relaxation time of PI. Thus, the high- ω plateau zone was too narrow to be resolved experimentally, and the PI chains relaxed almost immediately after their Rouse equilibration (retarded by PtBS). This PI relaxation activated the constraint release (CR) relaxation of PtBS to dilate the entanglement mesh for PtBS. A simple model considering the Rouse equilibration and CR/dilation processes described the G^* data of the blend surprisingly well, lending support to the molecular picture of the cooperative/simultaneous Rouse equilibration of the PI and PtBS chains. The model calculation was consistent with the rheo-optical data, which lent further support to this molecular picture.

Exact Algorithms for Computing the Tree Edit Distance between Unordered Trees

Akutsu, T.; Fukagawa, D.; Takasu, A.; Tamura, T., *Theoretical Computer Science*, **412**, 352-364 (2011).

Abstract

In this paper, we present a fixed-parameter algorithm for the edit distance problem for unordered trees under the unit cost model. The algorithm works in $O(2.62^k \cdot \text{poly}(n))$ time and $O(n^2)$ space, where the parameter k is the maximum bound of the edit distance and n is the maximum size of input trees. We also present polynomial time algorithms for the special case in which the maximum degree of the largest common subtree is bounded by a constant.